

09/ 93, 529

(FILE 'HOME' ENTERED AT 12:38:43 ON 17 DEC 2002)

FILE 'REGISTRY' ENTERED AT 12:38:56 ON 17 DEC 2002

L1 STRUCTURE UPLOADED  
L2 28 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:42:11 ON 17 DEC 2002

L3 9 S L2  
L4 0 S L3 AND (DISULF? OR DISULPH?)  
L5 0 S L3 AND PHOSPHIN?  
L6 0 S L3 AND ALKYLAT?

FILE 'REGISTRY' ENTERED AT 12:48:00 ON 17 DEC 2002

L7 1 S (136454-49-4)/RN  
L8 1 S (136454-32-5)/RN

FILE 'CAPLUS' ENTERED AT 12:49:04 ON 17 DEC 2002

L9 1 S L7 AND L8

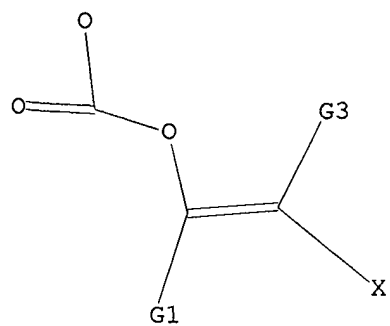
FILE 'STNGUIDE' ENTERED AT 12:50:54 ON 17 DEC 2002

FILE 'REGISTRY' ENTERED AT 12:51:39 ON 17 DEC 2002

=>

L1

STR



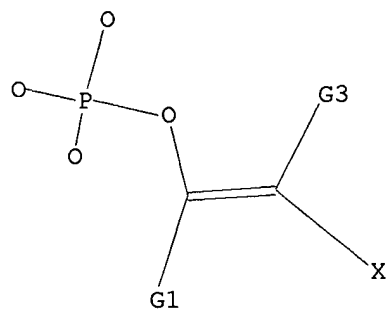
G1 Cb,Cy,Hy,Ak,H

G2 C,P

G3 Ak,Cb,Cy,Hy

L1

STR

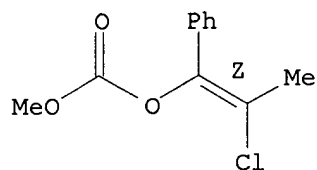


G1 Cb,Cy,Hy,Ak,H

G2 C, P

G3 Ak,Cb,Cy,Hy

Double bond geometry as shown.

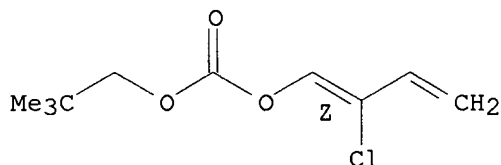


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 6 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 128728-52-9 REGISTRY  
CN Carbonic acid, 2-chloro-1,3-butadienyl 2,2-dimethylpropyl ester, (Z)-  
(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C10 H15 Cl O3  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

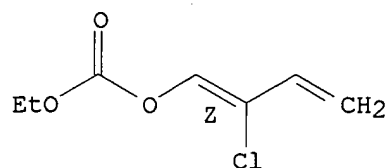


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 7 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 128728-51-8 REGISTRY  
CN Carbonic acid, 2-chloro-1,3-butadienyl ethyl ester, (Z)- (9CI) (CA INDEX  
NAME)  
FS STEREOSEARCH  
MF C7 H9 Cl O3  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

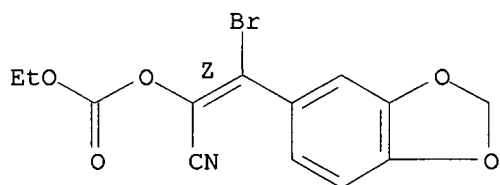


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 8 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-84-7 REGISTRY  
CN Carbonic acid, 2-(1,3-benzodioxol-5-yl)-2-bromo-1-cyanoethenyl ethyl ester, (Z)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C13 H10 Br N O5  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

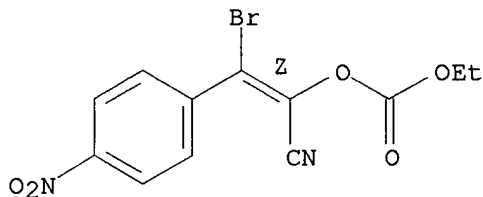


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 9 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-83-6 REGISTRY  
CN Carbonic acid, 2-bromo-1-cyano-2-(4-nitrophenyl)ethenyl ethyl ester, (Z)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C12 H9 Br N2 O5  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.



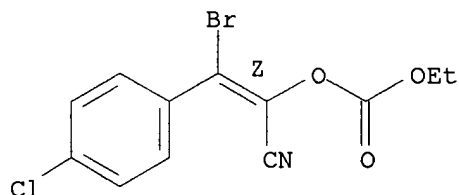
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 10 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-82-5 REGISTRY

CN Carbonic acid, 2-bromo-2-(4-chlorophenyl)-1-cyanoethenyl ethyl ester, (Z)-  
 (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C12 H9 Br Cl N O3  
 SR CA  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
 (\*File contains numerically searchable property data)

Double bond geometry as shown.

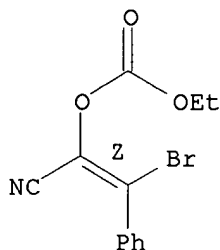


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 11 OF 28 REGISTRY COPYRIGHT 2002 ACS  
 RN 119420-81-4 REGISTRY  
 CN Carbonic acid, 2-bromo-1-cyano-2-phenylethenyl ethyl ester, (Z)- (9CI)  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C12 H10 Br N O3  
 SR CA  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
 (\*File contains numerically searchable property data)

Double bond geometry as shown.



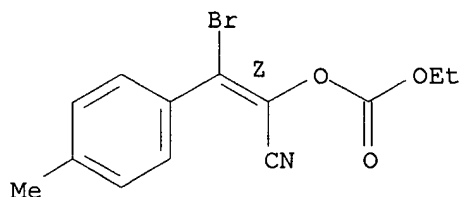
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 12 OF 28 REGISTRY COPYRIGHT 2002 ACS  
 RN 119420-80-3 REGISTRY  
 CN Carbonic acid, 2-bromo-1-cyano-2-(4-methylphenyl)ethenyl ethyl ester, (Z)-  
 (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C13 H12 Br N O3  
 SR CA  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)

Double bond geometry as shown.

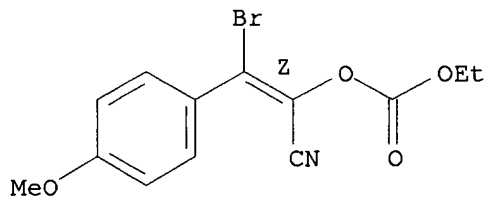


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 13 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-79-0 REGISTRY  
CN Carbonic acid, 2-bromo-1-cyano-2-(4-methoxyphenyl)ethenyl ethyl ester,  
(Z)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C13 H12 Br N O4  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

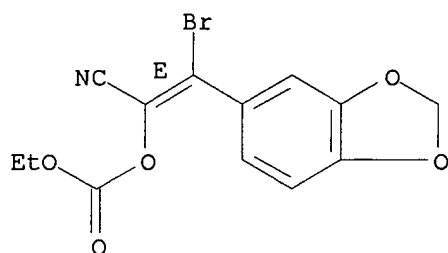


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 14 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-78-9 REGISTRY  
CN Carbonic acid, 2-(1,3-benzodioxol-5-yl)-2-bromo-1-cyanoethenyl ethyl  
ester, (E)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C13 H10 Br N O5  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

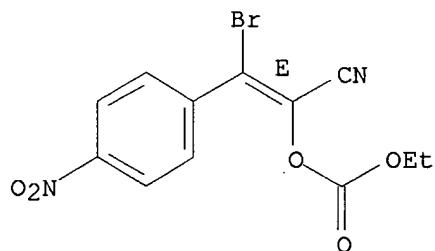


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 15 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-77-8 REGISTRY  
CN Carbonic acid, 2-bromo-1-cyano-2-(4-nitrophenyl)ethenyl ethyl ester, (E)-  
(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C12 H9 Br N2 O5  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.



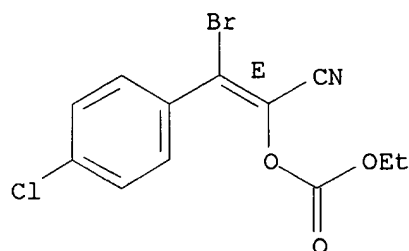
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 16 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-76-7 REGISTRY  
CN Carbonic acid, 2-bromo-2-(4-chlorophenyl)-1-cyanoethenyl ethyl ester, (E)-  
(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C12 H9 Br Cl N O3  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.



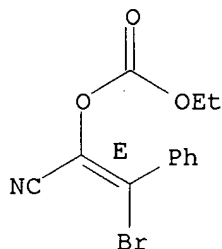


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 17 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-75-6 REGISTRY  
CN Carbonic acid, 2-bromo-1-cyano-2-phenylethenyl ethyl ester, (E)- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C12 H10 Br N O3  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

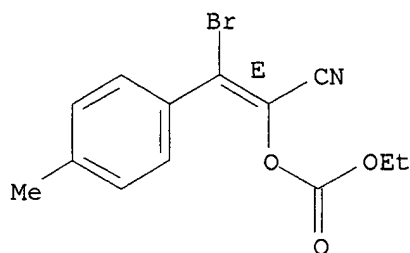


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 18 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-74-5 REGISTRY  
CN Carbonic acid, 2-bromo-1-cyano-2-(4-methylphenyl)ethenyl ethyl ester, (E)-  
(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C13 H12 Br N O3  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

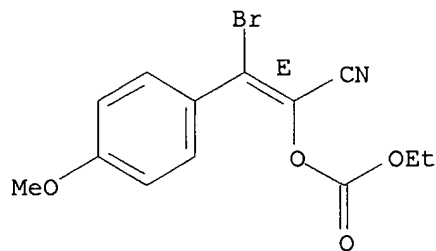


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 19 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 119420-73-4 REGISTRY  
CN Carbonic acid, 2-bromo-1-cyano-2-(4-methoxyphenyl)ethenyl ethyl ester,  
(E)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C13 H12 Br N O4  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

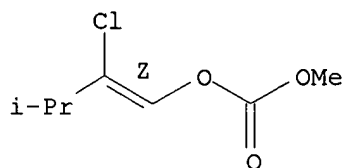


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 20 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 116432-05-4 REGISTRY  
CN Carbonic acid, 2-chloro-3-methyl-1-butenyl methyl ester, (Z)- (9CI) (CA  
INDEX NAME)  
FS STEREOSEARCH  
MF C7 H11 Cl O3  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

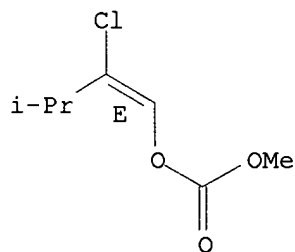


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 21 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 116432-04-3 REGISTRY  
CN Carbonic acid, 2-chloro-3-methyl-1-butenyl methyl ester, (E)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C7 H11 Cl O3  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

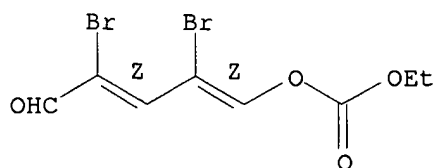


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 22 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 73093-08-0 REGISTRY  
CN Carbonic acid, 2,4-dibromo-5-oxo-1,3-pentadienyl ethyl ester, (Z,Z)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C8 H8 Br2 O4  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

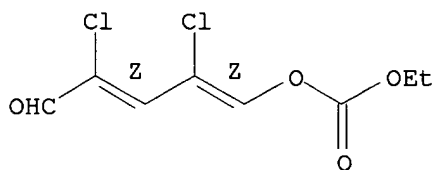


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 23 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 73093-07-9 REGISTRY  
CN Carbonic acid, 2,4-dichloro-5-oxo-1,3-pentadienyl ethyl ester, (Z,Z)-  
(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C8 H8 Cl2 O4  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

Double bond geometry as shown.

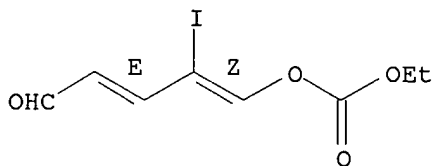


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 24 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 73093-06-8 REGISTRY  
CN Carbonic acid, ethyl 2-iodo-5-oxo-1,3-pentadienyl ester, (Z,E)- (9CI) (CA  
INDEX NAME)  
FS STEREOSEARCH  
MF C8 H9 I O4  
LC STN Files: CA, CAPLUS

Double bond geometry as shown.

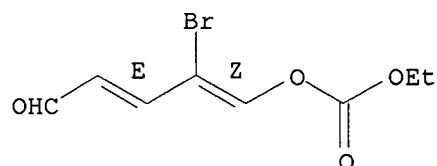


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 25 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 73093-04-6 REGISTRY  
CN Carbonic acid, 2-bromo-5-oxo-1,3-pentadienyl ethyl ester, (Z,E)- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C8 H9 Br O4  
LC STN Files: CA, CAPLUS

Double bond geometry as shown.

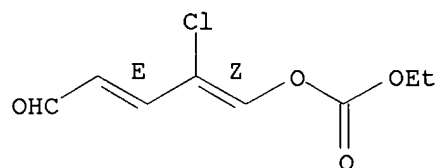


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 26 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 73093-02-4 REGISTRY  
CN Carbonic acid, 2-chloro-5-oxo-1,3-pentadienyl ethyl ester, (Z,E)- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C8 H9 Cl O4  
LC STN Files: CA, CAPLUS

Double bond geometry as shown.

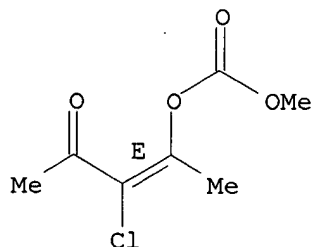


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 27 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 56578-59-7 REGISTRY  
CN Carbonic acid, 2-chloro-1-methyl-3-oxo-1-butenyl methyl ester, (E)- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C7 H9 Cl O4  
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)

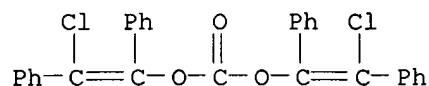
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 28 OF 28 REGISTRY COPYRIGHT 2002 ACS  
RN 26416-39-7 REGISTRY  
CN Carbonic acid, bis(2-chloro-1,2-diphenylvinyl) ester (8CI) (CA INDEX  
NAME)  
OTHER CA INDEX NAMES:  
CN .alpha.-Stilbenol, .alpha.'-chloro-, carbonate (2:1) (8CI)  
MF C29 H20 Cl2 O3  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER  
(\*File contains numerically searchable property data)

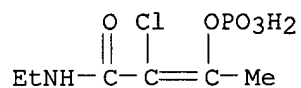


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS  
AN CA57:7553i CAOLD  
TI toxicology and pharmacology of a systemic phosphoric acid ester  
insecticide phosphamidon  
AU Jaques, Roland; Bein, H. J.  
IT 15844-87-8 **89490-23-3**

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS  
 RN **89490-23-3** REGISTRY  
 CN Crotonamide, 2-chloro-N-ethyl-3-hydroxy-, phosphate (7CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C6 H11 Cl N O5 P  
 LC STN Files: CAOLD



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
logD (LOGD)	-1.15	pH 1	(1) ACD
logD (LOGD)	-3.65	pH 4	(1) ACD
logD (LOGD)	-5.87	pH 7	(1) ACD
logD (LOGD)	-5.97	pH 8	(1) ACD
logD (LOGD)	-5.99	pH 10	(1) ACD
logP (LOGP)	-0.981+/-0.635		(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L		pH 1 (1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L		pH 4 (1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L		pH 7 (1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L		pH 8 (1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L		pH 10 (1) ACD
Molecular Weight (MW)	243.58		(1) ACD
pKa (PKA)	1.32+/-0.10	Most Acidic	(1) ACD

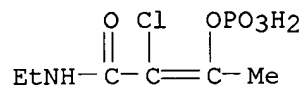
(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=>



L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS  
 RN 89490-23-3 REGISTRY  
 CN Crotonamide, 2-chloro-N-ethyl-3-hydroxy-, phosphate (7CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C6 H11 Cl N O5 P  
 LC STN Files: CAOLD



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
logD (LOGD)	-1.15	pH 1	(1) ACD
logD (LOGD)	-3.65	pH 4	(1) ACD
logD (LOGD)	-5.87	pH 7	(1) ACD
logD (LOGD)	-5.97	pH 8	(1) ACD
logD (LOGD)	-5.99	pH 10	(1) ACD
logP (LOGP)	-0.981+/-0.635		(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	243.58		(1) ACD
pKa (PKA)	1.32+/-0.10	Most Acidic	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=>

L2 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS  
AN CA57:7553i CAOLD  
TI toxicology and pharmacology of a systemic phosphoric acid ester  
insecticide phosphamidon  
AU Jaques, Roland; Bein, H. J.  
IT 15844-87-8 **89490-23-3**